Supplementary Materials

Inference of drug responses in cancer cells from cancer genomic features and compound chemical and therapeutic properties

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Legend

Fig S1

Correlating compound properties with drug response profiles. The boxplots show drugs with similar chemical features correlation well with IC50 profiles. X-axis indicates the correlations between drugs under their chemical and therapeutic properties, while y-axis indicates the correlations between drugs under their IC50 profiles. Barplots show the PCCs relating chemical property, target proteins, and ATC-codes with response profiles under IC50 measurement. It shows that drug responses correlate chemical property similarity more than other similarity measurements.

Fig S2

Precision-recall curves on each single data sources and their combinations. The precision-recall curves on each single data sources and their combinations are displayed with difference colors, it shows oncogene mutation and chemical properties are most predictive data sources, and expression and target protein might play trivial roles in prediction. The improved performance can be obtained by integrating all data sources of cells and drugs.

Fig S3

Assigning response value into three classes: sensitive, resistant and unknown. The left picture shows the distribution of IC50s across all 504 cell lines. Three kinds of bars are shown with different colors, and it determines three status of drug response: sensitivity, resistance and unknown relationship. The right picture is the heat map of relationship matrix. The horizontal axis represents drugs, and the vertical axis represents cell lines.

Drug sensitivity correlation vs. Correlation between chemical profiles: low, moderate, high. P<0.05

Drug sensitivity correlation vs. Correlation between ATC profiles: low, moderate, high

Drug sensitivity correlation vs. Correlation between targets profiles: low, moderate, high

Correlation Coefficient

Chem, Target, ATC

Precision vs. Recall

- Mut+Chem
- Mut+Target
- Mut+ATC
- CN+Chem
- CN+Target
- CN+ATC
- GE+Chem
- GE+Target
- GE+ATC
- Comb^c+Comb^d

Frequency vs. IC50

Compound / Cell line

Sensitivity   Unknown   Resistance